

On a Quaternionic Representation for $Sp(4, R)$

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Abstract

This work provides a quaternionic representation for real symplectic matrices in dimension four, analogous to that for the orthogonal group. It also provides a technique to compute this representation from the entries of the matrix being thus represented. As a byproduct it shows how one can compute the polar decomposition of a 4×4 symplectic matrix without any recourse to spectral calculations.

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1 Introduction

The most important groups in physics are, arguably, the rotation, and the symplectic groups, [1, 6]. In particular, the symplectic group is central to classical mechanics, [14], to classical and quantum optics, [1], quantum mechanics and quantum information processing, [3]. Therefore, having as many parametrizations of these groups as possible is desirable.

In dimension four, there is a well known parametrization of the orthogonal group via a pair of unit quaternions. This has innumerable applications in physics and engineering, [13, 15]. For the symplectic group, $Sp(4, R)$, there seems to be none. Note, by the “symplectic group”, we refer to the real symplectic group, and not the similarly named group $Sp(n)$, which preserves the standard inner product on H^n (here H stands for the quaternions). The latter is, of course, defined via quaternions, [15]. It is the intention of this note to provide such a parametrization for $Sp(4, R)$. Since the symplectic group is 10 dimensional (in comparison to the six dimensions of the $SO(4, R)$), the parametrization to be provided is accordingly more intricate.

For motivating the balance of the paper (in particular, the contents of the introductory section), we assume temporarily some familiarity with the algebra isomorphism between $H \otimes H$ (the tensor product of the quaternions, H , with itself) and the algebra of 4×4 real matrices, denoted $M_4(R)$, [15, 12, 5, 9, 16, 17, 19, 20]. See section 2 for more details. Using this algebra isomorphism, it would seem that to obtain a quaternion representation of an $X \in Sp(4, R)$, a logical approach would be to write out the conditions imposed on the quaternion representation of an $X \in M_4(R)$ by the relation

$$X^T J_4 X = J_4$$

where J_4 is the defining matrix of the symplectic group (its quaternion representation is $1 \otimes j$). However, this produces an immensely complicated system of equations.

Indeed, if one were to pursue this approach for the orthogonal group, i.e., write out the condition $X^T X = I$ in quaternion form, one does not recover the pair of unit quaternions representation. This is not surprising since those orthogonal matrices with determinant equal to -1 are not represented by decomposable tensors, i.e., by an element of $H \otimes H$, of the special form $u \otimes v$, with $u, v \in H$. Only if one were to insist that the quaternion representation of the

X one began with was to be already given by a decomposable tensor, would one recover the fact that an $X \in SO(4, R)$ is represented by a tensor $u \otimes v$, with u and v unit quaternions. Note that the condition, $\det(X) = 1$ for the group $SO(4, R)$ is subsumed by this representation, since the determinant of a matrix represented by $p \otimes q$, with $p, q \in H$, is

$$\|p\|^4 \|q\|^4$$

as a calculation shows.

However, it is not immediately evident that a special orthogonal matrix must be represented by a decomposable tensor. In our opinion, the simplest way to see this is to use the fact that the exponential map from $so(4, R)$ (the Lie algebra of 4×4 anti-symmetric matrices) is onto $SO(4, R)$. Since the quaternion representation of anti-symmetric matrices is easy to find (see section 2), a calculation, [19], shows that indeed matrices in $SO(4, R)$ must be represented by decomposable matrices. Unfortunately, the analogous statement, viz., that the exponential map from $sp(4, R)$ (the Lie algebra of Hamiltonian matrices) is onto $Sp(4, R)$, is false. Even if it were to be true, the exponential of Hamiltonian matrices do not typically admit a decomposable quaternion representation. Thus one cannot make the analogous simplification for the symplectic group.

To obtain a different perspective on the complexity of the question at hand, we note that it is straightforward to get quaternionic representations of Hamiltonian matrices. This is because: i) Hamiltonian matrices are expressible as $J_{2n}S$, with S real symmetric, and ii) quaternionic representations of symmetric matrices, and J_4 are easy to find. Now Hamiltonian matrices form the Lie algebra of symplectic matrices. So it is reasonable to inquire if a similar translation from orthogonal to symplectic matrices is valid. However, this is patently incorrect, i.e., it is not true that a symplectic matrix can be represented as J_4G , with G orthogonal. There also seems to be no easy modification of this approach which will do the job.

To understand, the approach taken in this work, we note that the initial suggestion that one write out the quaternionic version of the condition $X^T J_4 X = J_4$ leads to something tractable, provided one imposes the additional restriction that the original X be also *real symmetric*. This is very useful since it is known that in the polar decomposition $X = UP$,

of a symplectic X , both the orthogonal factor (U) and the positive definite factor (P) are symplectic as well (see [6, 14, 18], for instance). Since P is positive definite it is symmetric, and this explains the utility of starting with the assumption that X is symmetric and symplectic.

For a variety of reasons, it is more convenient to obtain quaternionic representations of symmetric and symplectic X and then further refine these to obtain quaternionic characterizations of positive definite and symplectic X . Therefore, we eschew one route to the latter, viz., using the fact that a positive definite symplectic X must be the exponential of a symmetric, Hamiltonian matrix (this exponentiation can be performed in closed form, [19] - but it would not yield the maximal benefit). Characterizing symplectic, orthogonal matrices is relatively easy. Combining the two one gets a quaternionic representation of symplectic matrices. These are stated in Theorem (3.1) and Theorem (3.4), with the latter being an improvement of the former which takes into account the characterization of positive definite, symplectic matrices obtained in Theorem (3.3) .

Let us now consider the question of finding formulae for these quaternions in terms of the entries of the given symplectic matrix X . The first step is to find P . Now P is not any arbitrary symplectic, positive definite matrix. It is, as in the case of all polar decompositions, the unique positive definite square root of $X^T X$. The traditional route to finding P involves diagonalizing $X^T X$ [see Remark (3.2)]. In this work we avoid this. Rather, we provide an explicit algorithm for finding P which requires only the solution of a very simple 2×2 linear system of equations. This is achieved by explicitly showing that there are only two real symmetric, symplectic matrices H , with positive trace, satisfying $H^2 = X^T X$. Since one of these must be P , we can easily find P . For all this it is crucial to characterize symmetric (not necessarily positive definite) symplectic matrices via quaternions, which explains the route chosen in this work. Of course, these results on symmetric, symplectic matrices are of independent interest. We note, however, that this work does indeed obtain a quaternionic characterization of positive-definite, symplectic matrices [see Theorem (3.4)]. In particular, a quaternionic parametrization of two-mode squeezing operators is thereby obtained, since positive-definite symplectic matrices are precisely those matrices which represent such operations, [1].

There are, of course, other global factorizations of the symplectic group, such as the Euler (Cartan) and Iwasawa decompositions, [1, 6, 7, 8, 21], which could have been used as starting

points for finding a quaternionic representation. But we found the polar decomposition as the most useful, since the polar decomposition of a matrix has innumerable applications, [10]. Thus, the fact that the polar decomposition based representation in this work, also yields a simple, constructive procedure for finding the polar decomposition itself as a byproduct played an important motivating role.

It is appropriate at this point to record some history of the linear algebraic applications of the isomorphism between $H \otimes H$ and $M_4(R)$. This isomorphism is central to the theory of Clifford algebras, [15]. However, it is only relatively recently been put into use for linear algebraic (especially numerical linear algebraic) purposes. To the best of our knowledge the first instance seems to be the work of [12], where it was used in the study of linear maps preserving the Ky-Fan norm. Then in [9], this connection was used to obtain the Schur canonical form explicitly for real 4×4 skew-symmetric matrices. Next, is the work of [5, 16, 17], wherein this connection was put to innovative use for solving eigenproblems of a variety of structured 4×4 matrices (including symmetric matrices). Finally, in [19, 20], this isomorphism was used to explicitly calculate the exponentials of a wide variety of 4×4 matrices.

The balance of this manuscript is organized as follows. In the next section some notation and preliminary results on symplectic matrices, positive definite matrices and the algebra isomorphism between $H \otimes H$ and $M_4(R)$ are collected. The next section contains all the results in this work. Proposition (3.1) provides the quaternion characterization of symmetric and symplectic matrices, central to this work. This is used in Theorem (3.1) to provide a quaternion representation of $Sp(4, R)$, which is further refined in Theorem (3.4). This refinement is based on a quaternionic characterization of positive definite matrices in Theorem (3.3). The principal technical tool in the proof of Theorem (3.3) is that of squaring a symmetric, symplectic matrix. This is also a key ingredient in the proof of Theorem (3.2). This latter theorem provides an explicit technique to calculate the polar decomposition of matrices in $Sp(4, R)$. While the proof of this theorem is somewhat lengthy, the key point is that it yields an algorithm for finding the positive definite factor in the polar decomposition, which requires only the calculation of a few inner products in R^3 and the solution of a 2×2 linear system. This is summarized in an algorithm. Next a different perspective is provided on the paucity

of symplectic, symmetric square roots of $X^T X$, for an $X \in Sp(4, R)$. As a byproduct an explicit formula for the characteristic polynomial of an $X \in Sp(4, R)$ is obtained. The final section offers some conclusions.

2 Notation and Preliminary Observations

The following definitions, notations and results will be frequently met in this work:

- $M_4(R)$ (also denoted $gl(4, R)$) is the algebra of real 4×4 matrices.
- J_{2n} is the $2n \times 2n$ matrix which, in block form, is given by $J_{2n} = \begin{pmatrix} 0_n & I_n \\ -I_n & 0_n \end{pmatrix}$.
 $Sp(2n, R)$ denotes the Lie group of symplectic matrices, i.e., those $2n \times 2n$ matrices, satisfying $X^T J_{2n} X = J_{2n}$. $sp(2n, R)$ is its Lie algebra, consisting of those real (resp. complex) $2n \times 2n$ matrices which satisfy $X^T J_{2n} + J_{2n} X = 0$. Such matrices are also called *Hamiltonian*.
- If $X \in Sp(2n, R)$, then $X^{-1} = -J_{2n} X^T J_{2n}$. Furthermore, if $X \in Sp(2n, R)$ then X^T is also in $Sp(2n, R)$.
- Essential use of the following theorem will be made in this work (see [6, 14, 18]):

Proposition 2.1 Let X be a real symplectic matrix, and let $X = PQ$ be its polar decomposition, with P positive definite and Q real orthogonal. Then P and Q are also real symplectic.

See [18] for examples of other matrix groups for which an analogous statement holds. It is worth recalling here that P is the unique positive definite square root of the positive definite matrix $X^T X$.

- For a polynomial $P(x) = \sum_{i=0}^n a_i x^i$, of degree at most n , its reverse is the polynomial $P_{rev}(x) = \sum_{i=0}^n a_{n-i} x^i$. In this work we will use the fact that the characteristic polynomial of a symplectic matrix *equals its reverse* [see [18], for instance]. This follows from the well-known fact that for any invertible matrix $m \times m$ A , with characteristic polynomial $p(x)$, the characteristic polynomial of A^{-1} is the polynomial

$(-1)^m(\det(A))^m x^m p(\frac{1}{x})$. Now for any polynomial, $x^m p(\frac{1}{x})$ is precisely its reverse. Further for symplectic A , m is even and $\det(A)$ is 1. Finally, a symplectic A is similar to its transpose. Hence, the characteristic polynomial of A is the same as that of its inverse, whence it equals its reverse.

We next collect some definitions and results on real positive definite matrices. All details, together with extensions to the complex positive semidefinite case, may be found in [10].

- **Definition 2.1** Let Y be a real positive definite matrix. A real square matrix Z satisfying $Y = Z^T Z$ is said to be a square root of Y .

See [10] for details (extending to the case of complex positive semidefinite matrices). Square roots of positive definite matrices are not unique. However, if Z_1 is a square root of Y then Z_2 is also a square root of Y iff there exists a real orthogonal matrix U such that $Z_2 = Z_1 U$.

- Let Y be a real positive definite matrix. Then there exist real symmetric matrices H such that $Y = H^2$. Clearly any such H is a square root in the sense of Definition (2.1).
- Let Y be a real positive definite matrix. Then there exists a unique real positive definite matrix P with $Y = P^2$. Clearly this P is an example of a real symmetric matrix whose square equals Y .

Next relevant definitions and results regarding quaternions and their connection to real matrices will be presented. Throughout H will denote the skew-field (the division algebra) of the *quaternions*, while P stands for the *purely imaginary* quaternions, tacitly identified with R^3 .

$H \otimes H$ and $M_4(R)$: The algebra isomorphism between $H \otimes H$ and $gl(4, R)$, which is central to this work is the following:

- Associate to each product tensor $p \otimes q \in H \otimes H$, the matrix, $M_{p \otimes q}$, of the map which sends $x \in H$ to $px\bar{q}$, identifying R^4 with H via the basis $\{1, i, j, k\}$. Thus, if $p =$

$p_0 + p_1i + p_2j + p_3k; q = q_0 + q_1i + q_2j + q_3k$, then

$$M_{p \otimes q} = \begin{pmatrix} u_0 & v_0 & w_0 & z_0 \\ u_1 & v_1 & w_1 & z_1 \\ u_2 & v_2 & w_2 & z_2 \\ u_3 & v_3 & w_3 & z_3 \end{pmatrix}$$

with

$$p\bar{q} = u_0 + u_1i + u_2j + u_3k$$

$$pi\bar{q} = v_0 + v_1i + v_2j + v_3k$$

$$pj\bar{q} = w_0 + w_1i + w_2j + w_3k$$

$$pk\bar{q} = z_0 + z_1i + z_2j + z_3k$$

Here, $\bar{q} = q_0 - q_1i - q_2j - q_3k$

- Extend this to the full tensor product by linearity, e.g., the matrix associated to $2(p_1 \otimes q_1) - 9(p_2 \otimes q_2)$ is the matrix $2M_{p_1 \otimes q_1} - 9M_{p_2 \otimes q_2}$. This yields an algebra isomorphism between $H \otimes H$ and $M_4(R)$.
- In particular, a basis for $gl(4, R)$ is provided by the sixteen matrices $M_{e_x \otimes e_y}$ as e_x, e_y run through $1, i, j, k$. Of these only $M_{1 \otimes 1}$ is not traceless. In particular, $J_4 = M_{1 \otimes j}$ belongs to this basis.
- Define conjugation in $H \otimes H$ by first defining the conjugate of a decomposable tensor $a \otimes b$ as $\bar{a} \otimes \bar{b}$, and then extending this to all of $H \otimes H$ by linearity. Furthermore $M_{\bar{a} \otimes \bar{b}} = (M_{a \otimes b})^T$.
- Thus, the most general element of $M_4(R)$ admits the quaternion representation $a1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k + s \otimes 1 + 1 \otimes t$, with $a \in R$ and $p, q, r, s, t \in P$. The summand $a1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k$ is the symmetric part of the matrix, while the summand $s \otimes 1 + 1 \otimes t$ is the skew-symmetric part of the matrix. Expressions for a, p, q, r, s, t (which are linear in the entries of the matrix being represented) are easy to find, [16]. Finally $4a$ is the trace of the matrix.

3 Quaternion Representations of $Sp(4, R)$

In this section the main results of this work are presented.

To develop a quaternionic representation of an $X \in Sp(4, R)$, let us invoke Theorem (2.1). Per that result it suffices to obtain quaternionic representations of positive definite, symplectic matrices and symplectic, orthogonal matrices.

Let $X = UP$ be the polar decomposition of X . Since U is symplectic and orthogonal it must, in fact, be special orthogonal. Obtaining the quaternionic representation of such a matrix is easy. It is given by $q = u \otimes v$, with u, v unit quaternions (corresponding to special orthogonality) with the further restriction that $vj = jv$ (corresponding to symplecticity). This imposes no further restriction on u , but forces v to be of the form $v = v_0 + v_2j$, with $v_0^2 + v_2^2 = 1$.

To obtain a quaternionic representation of P , it is convenient (for the reasons mentioned in Section 1) to obtain a quaternionic characterization of symmetric, symplectic X 's. This is achieved in:

Proposition 3.1 Let X be a 4×4 symplectic matrix which is also symmetric. Then it admits the quaternion representation $X = a1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k$, with $aq = r \times p$, $p.q = 0 = r.q$, and a satisfying the constraint $a^2 - p.p + q.q - r.r = 1$. If a , which is $\frac{1}{4}$ 'th the trace of X , is not zero then X is symplectic iff $aq = r \times p$ and $a^2 - p.p + q.q - r.r = 1$.

Proof: The proof proceeds by equating the quaternion expansion of $X^T J_4 X = X J_4 X$, viz., $(a 1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k)(1 \otimes j)(a 1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k)$ with $1 \otimes j$.

This calculation is facilitated by the observation that for any matrix X (not necessarily symplectic or symmetric), the matrix $X^T J_{2n} X$ is always skew-symmetric. Therefore, in the expansion $(a 1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k)(1 \otimes j)(a 1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k)$ one needs to inspect only those terms of the form $s \otimes 1$ and $1 \otimes t$, with $s, t \in P$ (i.e., those corresponding to the skew-symmetric terms) and equate all but one of them to zero. The non-zero term is, of course, the $1 \otimes j$ term and this is equated to 1. Specifically, expansion of $X^t J_4 X$ is

$$(a^2 - p.p + q.q - r.r)(1 \otimes j) + (2r \times p - 2aq) \otimes 1 + (2p.q)1 \otimes i + (2r.q)1 \otimes k$$

Note that the vanishing of the second term yields the condition $aq = r \times p$. Thus, if $a \neq 0$,

then either $q = 0$ or $q = \frac{r \times p}{a}$ and this, of course, ensures the conditions $p \cdot q = 0 = r \cdot q$. This finishes the proof.

Now note that for the situation at hand, where X is not merely symmetric but, in fact, positive definite we necessarily have $a \neq 0$. This yields a preliminary result about the quaternion representation of symplectic matrices, which will be refined later in this section:

Theorem 3.1 Let X be an element of $Sp(4, R)$. Then there exist $a, v_0, v_2 \in R$, $p, q, r \in P$, and a unit quaternion u satisfying the constraints $a^2 - p \cdot p + q \cdot q - r \cdot r = 1$, $q = \frac{r \times p}{a}$ and $v_0^2 + v_2^2 = 1$ such that X admits the following quaternion representation $X = [u \otimes (v_0 + v_2 j)][a \cdot 1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k]$.

Note that this result gives the correct dimension count for $Sp(4, R)$. u is determined by 3 real quantities and v_0, v_2 together yield one additional parameter. The non-compact portion of $Sp(4, R)$ is determined by the two vector quantities p, r , and the scalar a , with one restriction, thereby yielding 6 real parameters. Put together we get the dimension count to be 10.

We now turn to the issue of computing these quaternions from the entries of X . Assuming the symmetric portion of the representation is available, the calculation of the factor $[u \otimes (v_0 + v_2 j)]$ is amenable to the any technique which will yield the quaternion representation of a matrix in $SO(4, R)$. This ought to be folklore, but surprisingly the only explicit record of this that we were able to find is in [2].

Next, consider computing the symmetric, $[a \cdot 1 \otimes 1 + p \otimes i + \frac{r \times p}{a} \otimes j + r \otimes k]$ factor. This is, of course, not just any symmetric matrix. It is the unique positive definite square root of $X^T X$. To that end, one could, of course, resort to diagonalizing the symmetric matrix $X^T X$. Instead, as we will see below that there is an even more explicit method for finding the symmetric factor, which reveals some facts which are of interest in their own right.

Specifically, recall from Section 2, that any positive definite matrix is the square of a real symmetric matrix. The real symmetric matrix is not unique, but one of these is the unique positive definite square root of the positive definite matrix in question. Now, when the positive matrix is $X^T X$, $X \in Sp(4, R)$, we know that the unique positive definite square

root is also symplectic. Furthermore, being positive definite its trace is positive. So, instead of looking at all possible real symmetric matrices whose square is $X^T X$, one needs to inspect only those which are symplectic and have positive trace, in addition. One then finds the pleasant conclusion that there are only few such candidates.

Theorem 3.2 Let $X \in Sp(4, R)$. Then there are atmost two (and, at least one) matrices H which satisfy i) $H^2 = X^T X$; ii) H is real symmetric and symplectic; and iii) $\text{Trace}(H) > 0$. One of these is precisely the unique positive definite square root of $X^T X$, and thus the positive definite factor in the polar decomposition of X . Furthermore, H can be found explicitly via the solution of a simple linear systems.

Proof: Let $X \in Sp(4, R)$. Then so is X^T and hence $X^T X \in Sp(4, R)$. Let $b1 \otimes 1 + c \otimes i + d \otimes j + e \otimes k$ be its quaternion representation. Note, as $X^T X$ is positive definite, $b > 0$, while c, d, e are pure quaternions. Let H be a real symmetric, symplectic matrix with non-zero trace satisfying $H^2 = X^T X$. Suppose $H = a1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k$. Then equating H^2 to $X^T X$ yields the system of equations:

$$b = a^2 + p.p + q.q + r.r \quad (3.1)$$

$$c = 2ap + 2q \times r$$

$$d = 2aq + 2r \times p$$

$$e = 2ar + 2p \times q$$

In addition, as H is symplectic, this system is augmented by the conditions i) $a > 0$; ii) $q = \frac{r \times p}{a}$; iii) $1 = a^2 + q.q - p.p - r.r$.

The second equation in the system Equation (3.1), together with $2aq = r \times p$, yields $q = \frac{d}{4a}$. So, if we can find a (note, we know that a solution with $a > 0$ exists, in principle) then we obtain q .

At this point it is convenient to divide the argument into two cases. The case $q \neq 0$ and the case $q = 0$. Note (as $a \neq 0$) these are equivalent to the cases $d \neq 0$ and $d = 0$ respectively.

The case $d \neq 0$: To find a , it is first noted that H is symplectic, we have

$$1 = a^2 + q.q - p.p - r.r$$

and hence $\frac{b+1}{2} = a^2 + q \cdot q = a^2 + \frac{d \cdot d}{16a^2}$. This yields a quadratic for a^2 , viz.,

$$a^4 - \frac{b+1}{2}a^2 + \frac{d \cdot d}{16} = 0 \quad (3.2)$$

Note that the discriminant of the above equation is $\frac{(b+1)^2}{4} - \frac{d \cdot d}{4}$, and this is positive since $(b+1)^2 - d \cdot d = b^2 + 1 + 2b - d \cdot d$ can be expressed as $2b^2 + 2b - c \cdot c - e \cdot e$ (by using the fact that, $X^T X$ is symplectic and hence $b^2 + d \cdot d - c \cdot c - e \cdot e = 1$). But $2b^2 + 2b - c \cdot c - e \cdot e = b^2 + d \cdot d + 2b$ (since $b^2 - c \cdot c - e \cdot e = d \cdot d$). But $b^2 + d \cdot d + 2b > 0$, since b , being one-fourth the trace of the positive definite $X^T X$ is positive. Hence both its roots are real. Further, since its coefficients change sign ($\frac{b+1}{2}$ and $\frac{d \cdot d}{16}$ are positive) both these roots are positive. Pick any one root and let a be the positive square root of it. This yields a and hence q .

To find r and p , one inserts the expression $q = \frac{r \times p}{a}$ into the Equations for c and e and uses the vector triple product identities to find:

$$\begin{aligned} c &= 2ap + \frac{2}{a}[(r \cdot r)p - (p \cdot r)r] \\ e &= 2ar + \frac{2}{a}[(p \cdot p)r - (p \cdot r)p] \end{aligned} \quad (3.3)$$

This would yield a linear system for the unknowns p, r in terms of the knowns c and e provided we can express $p \cdot p, r \cdot r, p \cdot r$ in terms of e, c . To achieve this, first note that

$$\begin{aligned} c \cdot c &= 4a^2 p \cdot p + 4 \|q \times r\|^2 + 8a^2 p \cdot (q \times r) \\ e \cdot e &= 4a^2 r \cdot r + 4 \|p \times q\|^2 + 8a^2 r \cdot (p \times q) \end{aligned}$$

Hence,

$$c \cdot c - e \cdot e = 4a^2 p \cdot p - 4a^2 r \cdot r + 4 \|q \times r\|^2 - 4 \|p \times q\|^2$$

Next, using the identity $(u \times v) \cdot (\tilde{u} \times \tilde{v}) = (u \cdot \tilde{u})(v \cdot \tilde{v}) - (u \cdot \tilde{v})(\tilde{u} \cdot v)$, we find that

$$\|q \times r\|^2 = (q \cdot q)(r \cdot r)$$

(since $q \cdot r = 0$) and that

$$\|p \times q\|^2 = (p \cdot p)(q \cdot q)$$

(since $q \cdot p = 0$)

Thus

$$p.p - r.r = \frac{c.c - e.e}{4a^2 - 4q.q}$$

Since, we also know that $\frac{b+1}{2} = a^2 + q.q = 1 + p.p + r.r$, we have that

$$p.p + r.r = \frac{b-1}{2}$$

So, one gets a linear system for $p.p$ and $r.r$, in terms of already determined quantities. To find $p.r$, we compute that

$$c.e = (2ap + 2q \times r).(2ar + 2p \times q) = 4a^2(p.r) + 4(q \times r).(p \times q)$$

Hence,

$$c.e = 4a^2(p.r) + 4[(q.p)(r.q) - (q.q)(p.r)] = 4(a^2 - q.q)(p.r)$$

Now note that $a^2 - q.q \neq 0$. Indeed, if it was zero, then $a^2 = \frac{d.d}{16a^2}$. But recall, the quadratic for a^2 was $16a^4 + d.d = 16a^2 \frac{b+1}{2}$. So if $a^2 = \frac{d.d}{16a^2}$, this would then imply that $a^2 = \frac{b+1}{4}$, which is not true. So, we find $p.r = \frac{c.e}{4(a^2 - q.q)}$. This yields $p.r$.

Inserting these values for $p.p$, $p.r$ and $r.r$ into Equations (3.3) yields a linear system for the vectors p and r :

$$c = \alpha p + \beta r \tag{3.4}$$

$$e = \beta p + \gamma r$$

$$\text{with } \alpha = 2a + \frac{2r.r}{a} = 2a + \frac{b-1}{2a} + \frac{e.e - c.c}{a(4a^2 - 4q.q)}, \beta = -\frac{c.e}{4a^2 - 4q.q}, \gamma = 2a + \frac{2p.p}{a} = 2a + \frac{b-1}{2a} + \frac{c.c - e.e}{a(4a^2 - 4q.q)},$$

The system Equation (3.4) is readily solved. Indeed, the system is invertible as the Cauchy-Schwarz inequality reveals that the quantity $\alpha\gamma - \beta^2$ is at least $4a^2$.

Thus, we have found H . If this H is not positive definite, then the H corresponding to the other root of the Equation (3.2) has to be positive definite, since that is the only other H which is symplectic, symmetric, and with positive trace satisfying $H^2 = X^T X$.

The case $d = 0$ Now Equation (3.2), when $d = 0$ has two roots, viz., $\frac{b+1}{4}$ (which is strictly positive) and 0. Thus, by picking $a = \frac{\sqrt{b+1}}{2}$, $q = 0$, $p = \frac{c}{\sqrt{b+1}}$ and $r = \frac{e}{\sqrt{b+1}}$, we find the only

H which is symplectic, real symmetric, with positive trace and which satisfies $H^2 = X^T X$. Thus, by uniqueness, H must be the unique positive definite square root of $X^T X$.

In the constructive proof of the above theorem, a key step was an explicit formula for the trace of H^2 . This calculation can be used to obtain a complete characterization of positive definite symplectic X . Furthermore, it indicates which root of Equation (3.2) to pick to compute the desired H .

Theorem 3.3 Let $X = a(1 \otimes 1) + p \otimes i + q \otimes j + r \otimes k$ be a real symmetric, symplectic matrix. Then it is positive definite iff I) $a > 0$, II) $2a^2 - 2q.q + 1 > 0$. In particular, a symmetric and symplectic with matrix for which $a > 0, q = 0$ is positive definite.

Proof: It is well known that a real symmetric matrix is positive definite iff all its eigenvalues are positive. Let, $P_X(x) = x^n - a_{n-1}x^{n-1} + a_{n-2}x^{n-2} + \dots + (-1)^n a_0$ be the characteristic polynomial of X . Then, by Descartes' rule of signs, for instance, X is positive definite iff $a_i > 0$ for all $i = 0, \dots, n-1$. Since X is symplectic, in addition, its characteristic polynomial equals its reverse. Thus, we are guaranteed that $P_X(x)$ is of the form $P_X(x) = x^4 - a_3x^3 + a_2x^2 - a_1x + 1$. Now clearly $a_3 = \text{Tr}(X) = 4a$. It remains to find a_2 . Now, $a_2 = \frac{1}{2}[(\text{Tr}(X))^2 - \text{Tr}(X^2)]$. But $\text{Tr}(X^2) = 4(a^2 + q.q + p.p + r.r)$. Using, $1 = a^2 + q.q - p.p - r.r$, we see that $\text{Tr}(X^2) = 8a^2 + 8q.q - 4$. This yields,

$$P_X(x) = x^4 - 4ax^3 + (4a^2 - 4q.q + 2)x^2 - 4ax + 1$$

Hence positive definiteness of X is equivalent to $a > 0$ and $2a^2 - 2q.q + 1 > 0$. In particular if $a > 0$ and $q = 0$, X is positive definite.

From this follows a strengthening of Theorem (3.1), which is worth stating separately:

Theorem 3.4 Let $X \in Sp(4, R)$. Then there exist scalars a, v_0, v_2 , a unit quaternion u and pure quaternions p, q, r satisfying the constraints $a > 0, 2a^2 - 2q.q + 1 > 0, a^2 - p.p + q.q - r.r = 1, q = \frac{r \times p}{a}$ and $v_0^2 + v_2^2 = 1$ such that X admits the following quaternion representation $X = [u \otimes (v_0 + v_2j)][a 1 \otimes 1 + p \otimes i + q \otimes j + r \otimes k]$.

Remark 3.1 *Squeezing Transformations:* The authors of [1] argue persuasively that the most general squeezing transformation is given by (the metaplectic representation of) a positive-definite symplectic matrix. Thus, the above theorem obtains a quaternionic parametrization of such transformations for two-mode systems.

More generally, any application which requires the non-compact part of $Sp(4, R)$ would benefit from the parametrization in the above theorem, [1, 7, 8]. Note the matrices which are symplectic, *but not orthogonal* [i.e., the non-compact portion of $Sp(4, R)$] do *not* form a group. Hence, the polar decomposition is arguably the most economical fashion to extract the non-compact part of an $X \in Sp(4, R)$.

From Theorem (3.4), it is now clear which root of Equation (3.2) to pick for ensuring a positive definite H , when $d \neq 0$. Clearly, the larger a is, the smaller the $q.q$ is. Thus, the condition $2a^2 - 2q.q + 1 > 0$ is more likely to be satisfied by the candidate with the larger a . In fact, since there is precisely only one positive definite square root, the H corresponding to the larger value of a is positive-definite while the other candidate is not (this can also be directly verified). So one should pick the larger value for a , i.e., one should pick a to be the positive square root of $\frac{b+1}{2} + \sqrt{\frac{(b+1)^2}{4} - \frac{d.d}{4}}$.

We summarize the above discussion into an algorithm for finding the polar decomposition of an $X \in Sp(4, R)$:

- Algorithm 3.1**
- 1. Compute directly $X^T X$ - this is just the Gram matrix of the columns of X . $X^T X$ is positive definite (and thus symmetric) and is also symplectic.
 - 2. Compute the quaternion representation of $X^T X$. This is guaranteed to be of the form if $b(1 \otimes 1) + c \otimes i + d \otimes j + e \otimes k$ (with $b \in R, c, d, e \in P$) since $X^T X$ is symmetric. Furthermore, these quantities are linear in the entries of $X^T X$. In addition, b , which is $\frac{1}{4}$ the trace of $X^T X$, is positive.
 - 3. Let H be a matrix which has positive trace, real symmetric and symplectic, and which satisfies $H^2 = X^T X$. One such H is the positive definite factor in the polar decomposition of X . Let H , which is symmetric, have quaternion representation $a(1 \otimes 1) + p \otimes i + q \otimes j + r \otimes k$ (with $a \in R, p, q, r \in P$). Steps 4-6 below show how to compute a, p, q, r .
 - 4. If $d = 0$, then compute $a = \frac{\sqrt{b+1}}{2}$, $q = 0$, $p = \frac{c}{\sqrt{b+1}}$ and $r = \frac{e}{\sqrt{b+1}}$. This is guaranteed to be the positive factor in the polar decomposition of X .

- 5. If $d \neq 0$, then let a be the positive square root of the larger of the two strictly positive roots of the quadratic $x^2 - \frac{b+1}{2}x + \frac{d,d}{16} = 0$. Define $q = \frac{d}{4a}$. Find p, r by solving the linear system of equations Equation (3.4).
- 6. This yields H as the unique positive definite square root of $X^T X$ and thus the symmetric part of the polar decomposition of X .
- 7. Next compute XH^{-1} . For this no matrix inversion needs to be performed. Instead use the fact that $H^{-1} = -J_4 H^T J_4$. This shows that if

$$H = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

is the block-form of H , then

$$H^{-1} = \begin{pmatrix} D^T & -B^T \\ -C^T & A^T \end{pmatrix}$$

Thus, H^{-1} can be written by inspection. The matrix XH^{-1} is guaranteed to be symplectic and orthogonal, and thus will admit the quaternion representation $u \otimes (v_0 + v_2 j)$, with u a unit quaternion and $v_0^2 + v_2^2 = 1$.

- 8. To compute u, v_0, v_2 use the algorithm described in [2].

To give a different perspective on the “paucity” of symplectic, symmetric square roots of $X^T X$ when $d \neq 0$, a brief detour will be taken through a calculation which is relevant for Theorem (3.5) below as well.

Thus, suppose that H is a real symmetric, symplectic matrix with non-zero trace satisfying $H^2 = X^T X$, and suppose \tilde{H} is another. Then, since H, \tilde{H} are square roots of $X^T X$ [in the sense of Definition (2.1)], there exists a real orthogonal matrix U with $\tilde{H} = HU$. Clearly U must be symplectic too. Further the condition, $\tilde{H}^2 = H^2$ reads as $HUHU = HH$, which, since H is invertible, is equivalent to

$$UH = HU^T$$

Similarly, the condition that \tilde{H} be real symmetric is also equivalent to the same condition $UH = HU^T$. Indeed, $(HU)^T = HU$ is equivalent to $U^T H = HU$, which is equivalent to

$$H = UHU$$

This in turn, is equivalent to $UH = HU^T$.

So, considering H as fixed we examine which symplectic orthogonal U lead to $UH = HU^T$.

Let U be represented as $u \otimes v$. Recalling that the imaginary part of v is just $v_2 j$, we find that $UH = \alpha(1 \otimes 1) + \beta \otimes p + \gamma \otimes j + \delta \otimes k + s \otimes 1 + 1 \otimes t$, where the scalar α and the pure quaternions $\beta, \gamma, \delta, s, t$ are given by the equations

$$\alpha = au_0v_0 + (\text{Im } u.q)v_2 \quad (3.5)$$

$$\beta = u_0v_0p + v_0(\text{Im } u \times p) + u_0v_2r + v_2(\text{Im } u \times r) \quad (3.6)$$

$$\gamma = u_0v_0q + v_0(\text{Im } u \times q) + av_2\text{Im } u \quad (3.7)$$

$$\delta = -u_0v_2p - v_2(\text{Im } u \times p) + u_0v_0r + v_0(\text{Im } u \times r) \quad (3.8)$$

$$s = a(\text{Im } u)v_0 - u_0v_2q - v_2(\text{Im } u \times q) \quad (3.9)$$

$$t = -[v_0(\text{Im } u).p + v_2(\text{Im } u).r]\mathbf{i} + [au_0v_2 - v_0(\text{Im } u).q]\mathbf{j} + [v_2(\text{Im } u).p - v_0(\text{Im } u).r]\mathbf{k} \quad (3.10)$$

A similar calculation for HU^T reveals that the only non-zero terms in $UH - HU^T$ are the following:

- An $1 \otimes i$ term, viz., $-(2\text{Im}(u).p)v_0 - (2\text{Im}(u).r)v_2$.
- An $1 \otimes j$ term, viz., $2au_0v_2 - (2\text{Im}(u).q)v_0$.
- An $1 \otimes k$ term, viz., $2(\text{Im}(u)).pv_2 - 2(\text{Im}(u).r)v_0$.
- An $s \otimes 1$ term (with $s \in P$), viz., $2au_0\text{Im}(u) - 2u_0v_2q - 2v_2\text{Im}(u) \times q$.

Equating the first three terms to zero one finds that if $v_0 \neq 0$, then $\frac{v_2}{v_0} = -\frac{\text{Im}(u).p}{\text{Im}(u).r} = \frac{\text{Im}(u).r}{\text{Im}(u).p} = \frac{\text{Im}(u).q}{a\alpha_0}$.

This forces $\text{Im}(u).r = \text{Im}(u).p = v_2 = 0$ and $\text{Im}(u).q = 0$. Now as H is symplectic, with its q term and its trace is not zero, we have that q is proportional to $r \times p$. So $\text{Im}(u)$, being

perpendicular to p and q , must be parallel to q . But it is also orthogonal to q . So $\text{Im}(u) = 0$. Hence u is either $+1$ or -1 . Note that under these conditions the $s \otimes 1$ term also vanishes. Finally, $v_2 = 0$ forces v to be $+1$ or -1 . So, the only choices for $u \times v$, when $v_0 \neq 0$, are $1 \otimes 1$ or $-1 \otimes 1$.

If $v_0 = 0$, then one finds $\text{Im}(u).p = \text{Im}(u).r = 0$, again. Thus $\text{Im}(u)$ is proportional to q . Furthermore, as $a \neq 0$ and $v_2 \neq 0$, we get $u_0 = 0$. Thus, u is purely imaginary and proportional to q . Once again, the $s \otimes 1$ term vanishes under these conditions. Thus, the only choice for $u \times v$, in this case, are $\frac{q}{\|q\|} \otimes j$ or $-\frac{q}{\|q\|} \otimes j$.

Thus, there are precisely four symplectic, real symmetric square roots of $X^T X$ which have non-zero trace (two with positive trace, and the remaining two with negative trace). If H has positive trace, then it is easy to see (e.g., by inspecting the $1 \otimes 1$ term in \tilde{H}) that of the remaining three candidates only the one corresponding to $U = \frac{q}{\|q\|} \otimes j$ can also have positive trace.

Calculating the Characteristic Polynomial of a Symplectic X : We now show how to calculate the characteristic polynomial of a symplectic matrix, assuming its quaternion representation is available, without any need for a determinant calculation. Of course, calculating the quaternion representation is required. But since this provides the polar decomposition also, it seems worthwhile to pursue this route for the characteristic polynomial.

Thus, let X be symplectic, with $[u \otimes (v_0 + v_2 j)][a \ 1 \otimes 1 + p \otimes i + \frac{r \times p}{a} \otimes j + r \otimes k]$, its quaternion representation. This now reads as the expression

$$\alpha(1 \otimes 1) + \beta \otimes p + \gamma \otimes j + \delta \otimes k + s \otimes 1 + 1 \otimes t$$

The scalar α and the pure quaternions $\beta, \gamma, \delta, s, t$, have explicit expressions given by Equation (3.5), ..., Equation (3.10).

Since its characteristic polynomial $P_X(x)$ equals its reverse, it is of the form $P_X(x) = x^4 + a_3 x^3 + a_2 x^2 + a_1 x + 1$. Furthermore, $a_3 = -\text{Tr}(X)$ and $a_2 = \frac{1}{2}((\text{Tr}(X))^2 - \text{Tr}(X^2))$.

Clearly, then

$$a_3 = -4\alpha = -4(au_0 v_0 + (\text{Im } u.q)v_2) \quad (3.11)$$

To find a_2 one needs the trace of X^2 . *A useful observation here is that for this one does not need to calculate X^2 .* Once X has been found the trace of X^2 is simply $4(\alpha^2 + \beta.\beta +$

$$\gamma.\gamma + \delta.\delta - s.s - t.t).$$

Now an explicit calculation (which makes repeated use of the fact that u, v are unit quaternions) reveals $\alpha^2 + \beta.\beta + \gamma.\gamma + \delta.\delta - s.s - t.t$ is the expression

$$(v_0^2 - v_2^2)[q.q + (u_0^2 - \| \text{Im } u \|^2)a^2 - 2(\text{Im } u.q)^2] + p.p + r.r - 2[(\text{Im } u.p)^2 + (\text{Im } u.r)^2] + 8au_0v_0v_2(\text{Im } u.q)$$

Hence the expression for a_2 is

$$a_2 = 8a^2u_0^2v_0^2 + 8v_2^2(\text{Im } u.q)^2 + 2(v_2^2 - v_0^2)[q.q + (u_0^2 - \| \text{Im } u \|^2)a^2 - 2(\text{Im } u.q)^2] - 2(p.p + r.r) + 4[(\text{Im } u.p)^2 + (\text{Im } u.r)^2] \quad (3.12)$$

The above calculations can be summarized in

Theorem 3.5 Let $X \in Sp(4, R)$ be represented by quaternions as in Theorem (3.4). Then its characteristic polynomial is expressible as $P_X(x) = x^4 + a_3x^3 + a_2x^2 + a_3x + 1$, with a_3 and a_2 given by Equation (3.11) and Equation (3.12) respectively.

Remark 3.2 I) In computing the polar decomposition of a symplectic X , one could resort to first diagonalizing the symmetric matrix $X^T X$ in the form $V^T(X^T X)V = D$ (with V orthogonal) and then finding the unique positive definite square root, Y , in the form $Y = VD^{\frac{1}{2}}V^T$. Here $D^{\frac{1}{2}}$ is the diagonal matrix whose entries are the positive square roots of the entries of the diagonal matrix D . For this, one could use the method of [16], which uses quaternion methods for diagonalizing real symmetric 4×4 matrices. Recall that the key step (though not the sole step) in this is the following. Given a real symmetric matrix $\hat{a} \mathbf{1} \otimes \mathbf{1} + \hat{p} \otimes i + \hat{q} \otimes j + \hat{r} \otimes k$, one has to compute the singular value decomposition of the real 3×3 matrix $Z = [\hat{p} \ \hat{q} \ \hat{r}]$, i.e, the matrix whose columns are the vectors in R^3 equivalent to the pure quaternions $\hat{p}, \hat{q}, \hat{r}$. In this regard, it is noted that this calculation is somewhat simplified for the purpose at hand. Indeed, $X \in Sp(4, R)$ implies $X^T X \in Sp(4, R)$, i.e., the symmetric matrix $X^T X$ is also symplectic, and thus the corresponding terms $\hat{p}, \hat{q}, \hat{r}$ have the property that \hat{q} is orthogonal to \hat{p}, \hat{r} . So when computing the SVD of the corresponding Z , equivalently when forming the Grammian of the triple of vectors $\hat{p}, \hat{q}, \hat{r}$, one finds that

$$Z^T Z = \begin{pmatrix} \hat{p}.\hat{p} & 0 & \hat{p}.\hat{r} \\ 0 & \hat{q}.\hat{q} & 0 \\ \hat{p}.\hat{r} & 0 & \hat{r}.\hat{r} \end{pmatrix}$$

Hence finding the SVD amounts to just diagonalizing the 2×2 matrix

$$\begin{pmatrix} \hat{p} \cdot \hat{p} & \hat{p} \cdot \hat{r} \\ \hat{p} \cdot \hat{r} & \hat{r} \cdot \hat{r} \end{pmatrix}$$

This can be done by hand. However, partly because, finding the SVD of Z is not the sole step, this approach was eschewed in favour of Algorithm (3.1).

II) Computing the Euler-Cartan Decomposition of $Sp(4, R)$: The Euler-Cartan decomposition of $Sp(4, R)$ asserts that every $X \in Sp(4, R)$ can be factorized as $U_1 D U_2$, with U_i symplectic and orthogonal, for $i = 1, 2$, and D diagonal, positive-definite and symplectic. This factorization can be explicitly computed starting from the constructive polar decomposition given for $Sp(4, R)$ in this work. Indeed, let $X = UP$ be the polar decomposition. Following the technique in part I) of this remark, diagonalize the positive definite symplectic matrix P . It is simple and interesting to verify that the diagonalizing matrix V yielded by this procedure is actually symplectic and orthogonal. Thus, let $V^T P V = D$ be the diagonalization of P , with V symplectic and orthogonal, and D positive definite symplectic. This yields $X = U_1 D U_2$ with $U_1 = UV$, $U_2 = V^T$. Clearly the U_i are symplectic and orthogonal. This then yields (in closed form) the Euler-Cartan Decomposition of X .

4 Conclusions

This work produced a quaternionic representation for the symplectic group $Sp(4, R)$. Part of the utility of this work is that, in attempting to provide explicit formulae for this representation, one obtains a very simple and explicit technique for finding the polar decomposition of matrices in $Sp(4, R)$. Since the positive definite factor in this decomposition is one representation of the non-compact part of the symplectic group, this circumstance can be used to address applications where this factor is relevant, [1, 7, 8]. It would be an interesting exercise to derive other decompositions of $Sp(4, R)$ starting from the representation provided here.

Finding similar quaternionic representations of matrix groups preserving other bilinear forms in dimension four is an interesting question. It remains to see whether these lead to as elegant a set of expressions, such as those for the symplectic group. Indeed, it is no exaggeration to say that a pivotal role in the results here is played by the fact that the q term, in both Theorem (3.1) and Theorem (3.4), is essentially the cross product of the r

and p terms. Extending such representations to higher dimensions is also open. Quaternionic representations are, of course, limited to dimension four, just as there is no similar extension of the pair of unit quaternions representation to higher dimensional orthogonal groups. However, one can hope that in conjunction with either numerical techniques for the symplectic group, [4] or methods of Clifford Algebras, [15] these results can be extended to higher dimensions.

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